Monte Carlo Solution of a Spatially-Discrete Transport Equation Part II: Diffusion and Transport/Diffusion

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Abstract

We introduce a particle-based hybrid method where Monte Carlo particles are continuous in angle, but traverse discrete space in a diffusion sense. According to the sampling of a diffusion solution, a particle born in, or entering, a cell either gets absorbed inside the cell or leaks out one of the cell faces. This Discrete Diffusion Monte Carlo (DDMC) method is very similar to the S_∞ method, where Monte Carlo particles traverse discrete space in a transport sense. In fact, we couple the two hybrid methods to get a particle-based Multi-Hybrid method, where the particle events in a particular cell are determined either by a diffusion solution or a transport solution, whichever is appropriate. The Multi-Hybrid method allows for both resolution of transport boundary layers and time savings in diffusive regions. We show results for mono-energetic neutron transport, with isotropic scattering and sources, in one-dimensional slab geometry. The DDMC results agree well with deterministic diffusion. The multi-hybrid method agrees well with deterministic transport and shows improved efficiency over the pure S_∞ method by factors of 3 and 8.

1 Introduction and Motivations

We develop the Discrete Diffusion Monte Carlo (DDMC) method for mono-energetic neutron transport with isotropic scattering and isotropic sources in one-dimensional slab geometry. The method considers Monte Carlo particles that are continuous in angle, but travel in discrete space. When a particle is born in, or enters, a cell, we solve a cell-centered discrete diffusion equation for that cell. We interpret the diffusion solution probabilistically to determine absorption and leakage probabilities in the cell. Thus, a particle travels from cell-face to cell-face until it is absorbed or escapes the system.

DDMC is very similar to the S_∞ method [Urbatsch, Morel, and Gulick, 1999] where particles traverse discrete space according to lumped, linear-discontinuous (LLD) discrete transport. Since both methods are particle-based, we find that we can spatially couple them to achieve a particle-based Multi-Hybrid method that allows us to use transport where required and diffusion where possible.

The immediate motivation for the DDMC method is to speed up transport calculations. Additionally, the DDMC method is a candidate for investigating residual methods, through which Monte Carlo solutions of linear systems of equations can achieve exponential convergence [Halton, 1994].

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DDMC is faster than particle-based transport methods, but only as accurate where the diffusion approximation applies. DDMC's advantage over deterministic diffusion is that, in constructing hybrid transport/diffusion methods, it easily couples spatially to particle-based transport. In the realm of thermal radiative transfer, at least three hybrid transport/diffusion methods have been published. Pomraning and Foglesong [Pomraning and Foglesong, 1979] couple transport and diffusion with a modified Marshak boundary condition. DDMC's potential advantage over their method is that it would allow time-implicitness, whereas theirs would not because of probable time decoupling between the transport and diffusion. N'Kaoua [N'Kaoua, 1991] published a matrix hybrid method that allows for full time-implicitness, but requires storage of large matrices. Fleck and Canfield's [Fleck and Canfield, 1984] "Random Walk" allows particles to diffuse to the outer edge of a sphere centered about their location. The Random Walk occurs only within cells when the diffusion approximation applies and turns itself off near the outer edges of cells. Thus, if DDMC was applied to radiative transfer, its cell-face to cell-face transport would be faster than the Random Walk. Of these methods, the Random Walk is the only one that automates where and when diffusion is used. However, this automation in the Random Walk is intimately tied to the spatial discretization. The other schemes, including ours, have no automation as to when and where to turn on the diffusion.

2 Diffusion Approximation

We begin with the neutron transport equation in one-dimensional slab geometry, with isotropic scattering, one energy group, and isotropic internal sources,

$$\mu \frac{\partial \psi(x,\mu)}{\partial x} + \sigma_t(x)\psi(x,\mu) = \frac{\sigma_s(x)}{2}\phi(x) + \frac{q(x)}{2} \quad , \tag{1}$$

where μ is the cosine of the polar angle, $x \in [0, X]$ is the spatial variable, $\psi(x,\mu)$ is the angular flux, $\sigma_t(x)$ is the total cross section, $\sigma_s(x)$ is the scattering cross section, $q(x)$ is the isotropic, internal source, and $\phi(x)$ is the scalar flux:

$$\phi(x) = \int_{-1}^{1} \psi(x,\mu)\, d\mu \quad . \tag{2}$$

The boundary conditions are that the incoming angular fluxes are specified,

$$\psi(0,\mu) = f(\mu) \quad , \quad \mu > 0 \quad , \tag{3}$$

$$\psi(X,\mu) = g(\mu) \quad , \quad \mu < 0 \quad . \tag{4}$$

The corresponding diffusion equation and boundary condition are

$$-\frac{d}{dx}D(x)\frac{d}{dx}\phi(x) + \sigma_a(x)\phi(x) = q(x) \quad , \quad x \in S \quad , \tag{5}$$

and

$$4J^{-}(x) = \phi(x) + 2D(x)\frac{d\phi(x)}{dx}\mathbf{n}\cdot\mathbf{i} \quad , \quad x \in \partial S \quad , \tag{6}$$

where $D(x)$ is the diffusion coefficient,

$$D = \frac{1}{3\sigma_t(x)} \quad , \tag{7}$$

$\sigma_a(x) = \sigma_t(x) - \sigma_s(x)$ is the absorption cross section, S is in the interior of the system, $J^-(x)$ is the partial incoming current, ∂S is the system boundary, $\mathbf{n}$ is an outward unit normal, and $\mathbf{i}$ is the unit normal in the positive x-direction [Bell and Glasstone, 1985]. The relationship between the net current and the partial currents is as follows:

$$\begin{aligned} J(x) &= \int_{-1}^{1} \mu\psi(x,\mu)\, d\mu = \int_{-1}^{0} \mu\psi(x,\mu)\, d\mu + \int_{0}^{1} \mu\psi(x,\mu)\, d\mu \\ &= -\int_{-1}^{0} |\mu|\psi(x,\mu)\, d\mu + \int_{0}^{1} |\mu|\psi(x,\mu)\, d\mu = \begin{cases} -J^+(x) + J^-(x) & \text{for } \mathbf{n} = \text{-}\mathbf{i} \\ -J^-(x) + J^+(x) & \text{for } \mathbf{n} = \mathbf{i} \end{cases} \quad . \end{aligned} \tag{8}$$

We also have Fick's Law,

$$J(x) = -\frac{1}{3\sigma_t}\frac{d\phi(x)}{dx} \quad , \tag{9}$$

which comes from the first angular moment of the transport equation assuming the angular flux is linear in μ.

3 Discrete Diffusion

We consider diffusion on a single cell of width Δx and outward normals $\mathbf{n}$, as shown in Fig. 1. We wish to obtain discrete expressions for the continuous expressions of Fick's Law, the Marshak boundary conditions, and the net current. For quantities such as flux and current, the subscript "L" refers to the left edge of the cell, "R" refers to the right edge of the cell, and "C" refers to the center of the cell.

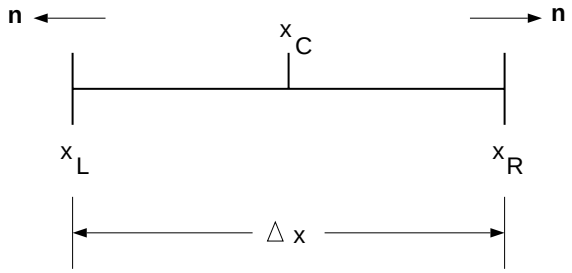

Figure 1: A single cell of width Δx and outward normals, $\mathbf{n}$.

First, we operate on the diffusion equation by $\int_{x_L}^{x_R}(\cdot)dx$ to produce a net balance equation

$$J_R - J_L + \sigma_a \phi_C \Delta x = q_C \Delta x \quad , \tag{10}$$

where the cross section is constant within a cell, and

$$q_C = \frac{1}{2}(q_L + q_R) \quad . \tag{11}$$

From Fick's Law, Eq. (9), we write the discrete, cell edge net currents,

$$J_L = -\frac{2D}{\Delta x}(\phi_C - \phi_L) \tag{12}$$

$$J_R = -\frac{2D}{\Delta x}(\phi_R - \phi_C) \quad . \tag{13}$$

Evaluating the Marshak boundary condition, Eq. (6), at each cell edge gives two discrete expressions for the partial incoming currents,

$$J_L^- = -\frac{D}{\Delta x}\phi_C + \left(\frac{1}{4} + \frac{D}{\Delta x}\right)\phi_L \quad , \tag{14}$$

$$J_R^- = -\frac{D}{\Delta x}\phi_C + \left(\frac{1}{4} + \frac{D}{\Delta x}\right)\phi_R \quad . \tag{15}$$

From Eq. (8), we evaluate the net current at the cell edges and obtain

$$J_L = -J_L^+ + J_L^- \quad , \tag{16}$$

$$J_R = J_R^+ - J_R^- \quad . \tag{17}$$

Equations (10) and (12) through (17) constitute seven equations in the seven unknowns, ϕ_C, ϕ_L, ϕ_R, J_L, J_R, J_L^+, and J_R^+. Before solving for these unknowns, we use the definitions of the net current in the balance equation to get a detailed balance equation,

$$J_L^+ + J_R^+ + \sigma_a\phi_C\Delta x = J_L^- + J_R^- + q_C\Delta x \quad , \tag{18}$$

which says that what enters a cell is equal to the sum of what exits the cell and what is absorbed in the cell. The DDMC method is based on this detailed balance equation.

Since we will not use ϕ_L and ϕ_R explicitly in the DDMC method, we eliminate them between the discrete Marshak boundary conditions and the discrete Fick's Law. Specifically, we solve the Marshak equations, Eqs. (14) and (15), for ϕ_L and ϕ_R, respectively, and substitute into the discrete Fick's Law equations, Eqs. (12) and (13), to obtain expressions for the net currents at the cell edges,

$$J_L = \frac{8D}{\Delta x + 4D}J_L^- - \frac{2D}{\Delta x + 4D}\phi_C \quad , \tag{19}$$

$$J_R = -\frac{8D}{\Delta x + 4D}J_L^- + \frac{2D}{\Delta x + 4D}\phi_C \quad . \tag{20}$$

We may find an expression for the cell-center scalar flux by using the discrete net current equations, Eqs. (19) and (20), in the net balance equation, Eq. (10):

$$\phi_C = \frac{8D}{4D + \sigma_a\Delta x(\Delta x + 4D)}\left(J_L^- + J_R^-\right) + \frac{(\Delta x + 4D)}{4D + \sigma_a\Delta x(\Delta x + 4D)}q_C\Delta x \quad . \tag{21}$$

We can also use the discrete net current equations, Eqs. (19) and (20), with the definitions of the net currents, Eqs. (16) and (17), to get expressions for the partial exiting currents,

$$J_L^+ = \frac{2D}{\Delta x + 4D}\phi_C + \frac{\Delta x - 4D}{\Delta x + 4D}J_L^- \quad , \tag{22}$$

$$J_R^+ = \frac{2D}{\Delta x + 4D}\phi_C - \frac{\Delta x - 4D}{\Delta x + 4D}J_R^- \quad . \tag{23}$$

Therefore, we can calculate the cell-center scalar flux, ϕ_C, from Eq. (21) and the partial exiting currents, J_L^+ and J_R^+, from Eqs. (22) and (23) and use them in the detailed balance equation, Eq. (18).

4 Discrete Diffusion Monte Carlo

In the DDMC method, we begin particles with a nominal weight of unity. (The normalization due to source particle apportionment may, however, produce particle weights slightly different than unity.) The right hand side of the balance equation, Eq. (18), is the cell's source, which includes incoming partial currents and internal sources. We consider one analog particle at a time, so only one of the three source elements will be nonzero. Upon sampling the type and location of a source particle, we relate the particle weight, wt, to the discrete diffusion source values in the following manner:

$$\begin{aligned} J_L^- &= \begin{cases} wt & \text{if entering cell from the left} \\ 0 & \text{otherwise} \end{cases} \\ J_R^- &= \begin{cases} wt & \text{if entering cell from the right} \\ 0 & \text{otherwise} \end{cases} \\ q_C \Delta x &= \begin{cases} wt & \text{if born in the cell} \\ 0 & \text{otherwise} \end{cases} \end{aligned} \quad . \tag{24}$$

We note that we can equate the particle weight to the total discrete source in the cell,

$$wt \equiv J_L^- + J_R^- + q_C \Delta x \quad , \tag{25}$$

since only one of the three terms is nonzero at any given time.

In order to determine the next event that the source particle undergoes, we divide Eq. (18) through by the right hand side to get

$$\frac{J_L^+}{J_L^- + J_R^- + q_C \Delta x} + \frac{J_R^+}{J_L^- + J_R^- + q_C \Delta x} + \frac{\sigma_a \phi_C \Delta x}{J_L^- + J_R^- + q_C \Delta x} = 1 \quad . \tag{26}$$

Setting the probability of leakage out the left side of the cell, $P_{leak\ left}$, as

$$P_{leak\ left} = \frac{J_L^+}{J_L^- + J_R^- + q_C \Delta x} \quad , \tag{27}$$

setting the probability of leakage out the right side of the cell, $P_{leak\ right}$, as

$$P_{leak\ right} = \frac{J_R^+}{J_L^- + J_R^- + q_C \Delta x} \quad , \tag{28}$$

and setting the probability of absorption in the cell, P_{abs}, as

$$P_{abs} = \frac{\sigma_a \phi_C \Delta x}{J_L^- + J_R^- + q_C \Delta x} \quad , \tag{29}$$

we obtain the following probability equation,

$$P_{leak\ left} + P_{leak\ right} + P_{abs} = 1 \quad . \tag{30}$$

To determine these probabilities, we use the appropriate source from Eq. (24) in Eq. (21) to determine the cell-center flux, ϕ_C. Then we use Eqs. (22) and (23) to get the partial exiting currents out each

side. Once the probabilities are calculated from Eqs. (27) to (29), we sample the particle's next event. If the particle is absorbed, its life is over. If the particle escapes the cell, we check if it escapes the system. If not, we sample its new direction from a cosine distribution,

$$\mu = \sqrt{\xi} \quad , \tag{31}$$

where $\xi \in (0,1)$ is a new random number. This distribution neglects the anisotropic term in the angular flux, which is assumed linear in μ in the diffusion approximation. (Although the particle's direction is not really necessary for DDMC, we retain it in order to facilitate the coupling to S_∞, which is discussed in the next section.) Every time we solve the diffusion equation in a cell, we accumulate the cell-center flux. We also obtain the cell-edge scalar fluxes from each diffusion solution by using the discrete Marshak boundary conditions in Eqs. (14) and (15). At the end of the calculation, we divide by the total weight of source particles to get an estimate of the overall scalar fluxes.

5 Multi-Hybrid Method

Both the DDMC method and the S_∞ method [Urbatsch, Morel, and Gulick, 1999] are particle-based methods. In each method, the cells do not explicitly depend on one another. A particle, upon entering a cell, does not care if its discrete position is determined by a diffusion calculation or a transport calculation. Therefore, we may mix the two hybrid methods to produce a Multi-Hybrid method. In cells where diffusion is not a good approximation—where transport effects exist—we should use S_∞. In cells where diffusion is valid, we may use DDMC. Overall, then, in one calculation, the transport gives us the accuracy we need where we need it, and diffusion gives us a faster calculation. The selection of the transport/diffusion boundary is not automatic. It should be chosen somewhat into the diffusive region to ensure that the diffusion approximation is not used in a transport region.

Although we do not show it here, DDMC would couple to regular Monte Carlo just as well as it does to S_∞.

6 Results

We first compare DDMC to cell-centered discrete diffusion because they should be equivalent. We also compare the Multi-Hybrid results to discrete-ordinates S_{32} results. Finally, we report the speedup that the Multi-Hybrid method provides over S_∞ for both a boundary problem and an internal source problem.

6.1 Purely Scattering Slab

The system we consider here is a purely scattering slab that is 100 mean free paths (mfp) thick. A normal, or nearly-normal, flux is incident on the left side of the slab.

We compare DDMC results to those of a deterministic, cell-centered diffusion calculation. The purely scattering slab has 100 cells, each one mfp thick. Here, the incident flux is exactly normal. Figure 2 shows that the scalar fluxes for DDMC and cell-centered deterministic diffusion agree very well. The coverage rates were tighter than expected: 79% were within one standard deviation and 100% were within two standard deviations. (The expected coverage rates are, respectively, 67% and 95%.)

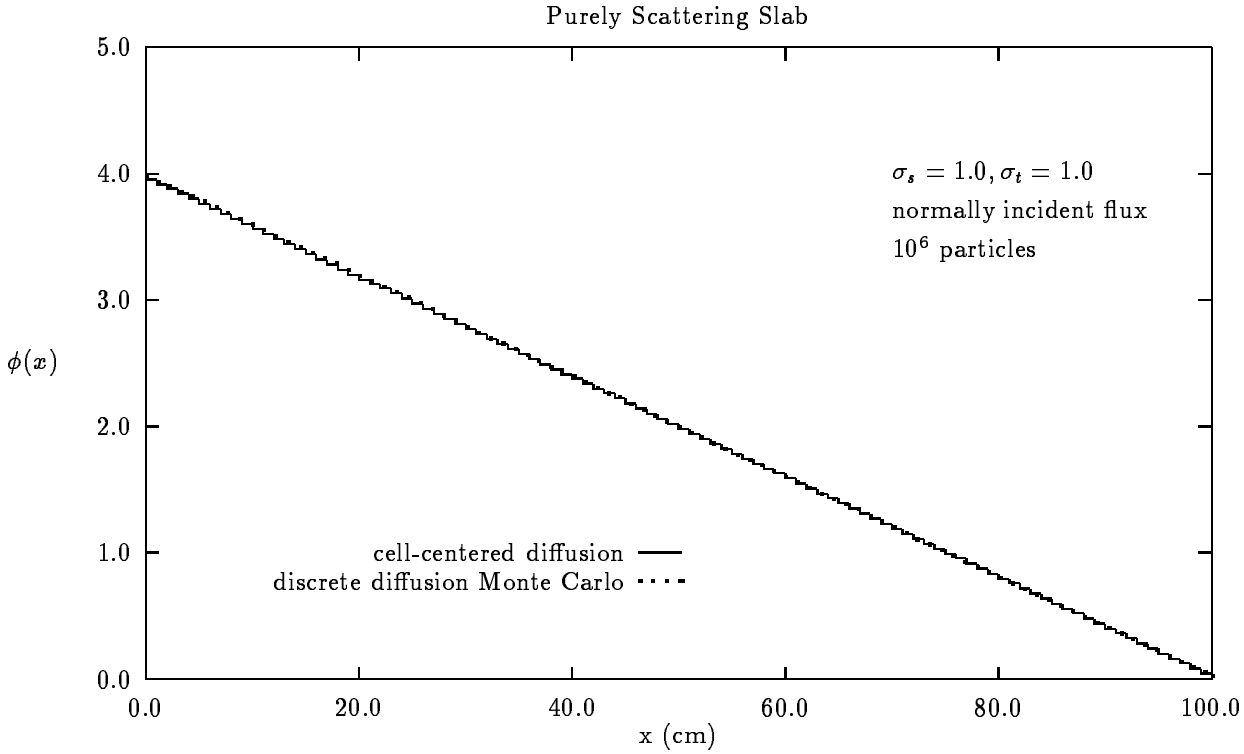

Figure 2: DDMC and deterministic, cell-centered diffusion results for a 100-mfp thick, purely scattering slab with a normally incident flux on the left side.

Figure 3 shows the cell-centered deterministic diffusion scalar flux, the deterministic S_{32} scalar flux, and, for comparison, the S_∞ scalar flux. In this problem, the nearly normally incident flux induces transport boundary-layer effects that diffusion simply cannot resolve. Although diffusion cannot resolve the boundary layer, it is a good approximation in the interior of this problem.

Thus, we are motivated to use transport in the boundary layer and diffusion in the interior. With one calculation, we use S_∞ in the first 5 cells (one mfp each) and DDMC in the remaining 95 cells (one mfp each). Since we do not need all the spatial resolution in the diffusion region, we run another set of calculations, maintaining the 5 S_∞ cells in the boundary layer, but using only one 95-mfp-thick diffusion cell in the rest of the slab. We also run this 6-cell problem with S_∞ only. Since we are comparing our results to deterministic S_{32} results, the direction cosine of the incident angle is 0.99726386184982, which is the cosine closest to normal in the S_{32} quadrature. The results for both Multi-Hybrid calculations are shown in Fig. 4 along with the S_{32} result. The agreement is excellent.

In order to quantitatively analyze the various methods, we use the figure of merit, FOM,

$$\text{FOM} = \frac{1}{R_{max}^2 t_{cpu}} \quad , \tag{32}$$

where t_{cpu} is the cpu time in seconds on a SGI Octane, and R_{max}^2 is the square of the maximum relative statistical error in the scalar flux over all left and right cell values.

The timings and figures of merit for the hybrid and Multi-Hybrid calculations are shown in Table 1.

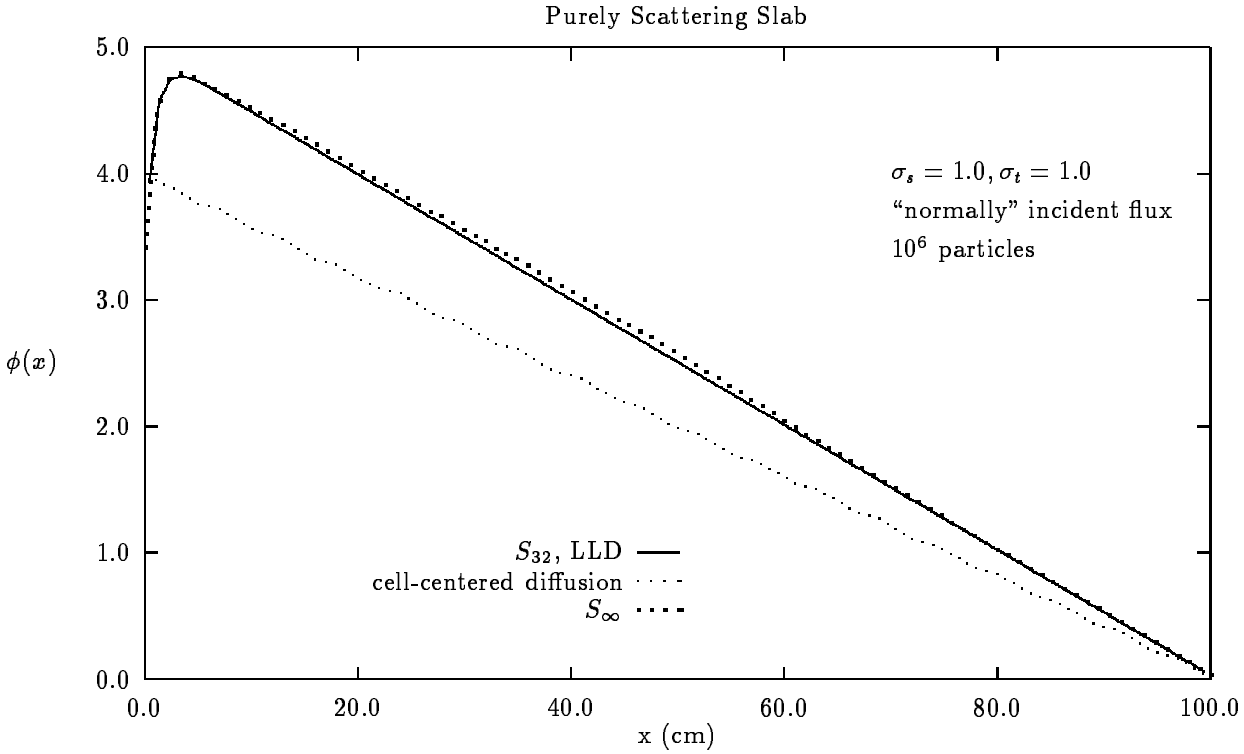

Figure 3: The normally incident flux has transport effects that diffusion cannot handle, as shown by the deterministic cell-centered diffusion scalar flux and the discrete ordinates S_{32} scalar flux.

DDMC is the fastest. However, DDMC alone does not resolve the boundary layer. The other calculations use S_∞ in the first five cells and thus resolve the boundary layer. For the 100-cell calculations, we see that the Multi-Hybrid method has an FOM about 2.7 times larger than that of S_∞. In the problems that used more judicious zoning, the Multi-Hybrid method had a factor of 8 improvement in the FOM.

Table 1: CPU times and figures of merit for the hybrid and Multi-Hybrid methods on the purely scattering slab, each using 10^6 particles.

Method	number of cells transport/diffusion	t_{cpu} (s)	FOM	qualitative result
DDMC	0/100	466	14.5	"diffusion"
S_∞	100/0	1573	4.67	"transport"
S_∞ / DDMC	5/95	667	12.7	"transport"
S_∞	6/0	1045	141	"transport"
S_∞ / DDMC	5/1	151	1137	"transport"

6.2 Internal Source Problem

Our second test problem, from McCoy and Larsen [McCoy and Larsen, 1971], models half of a slab reactor composed of iron and water with a reflecting boundary condition on the left side. The problem

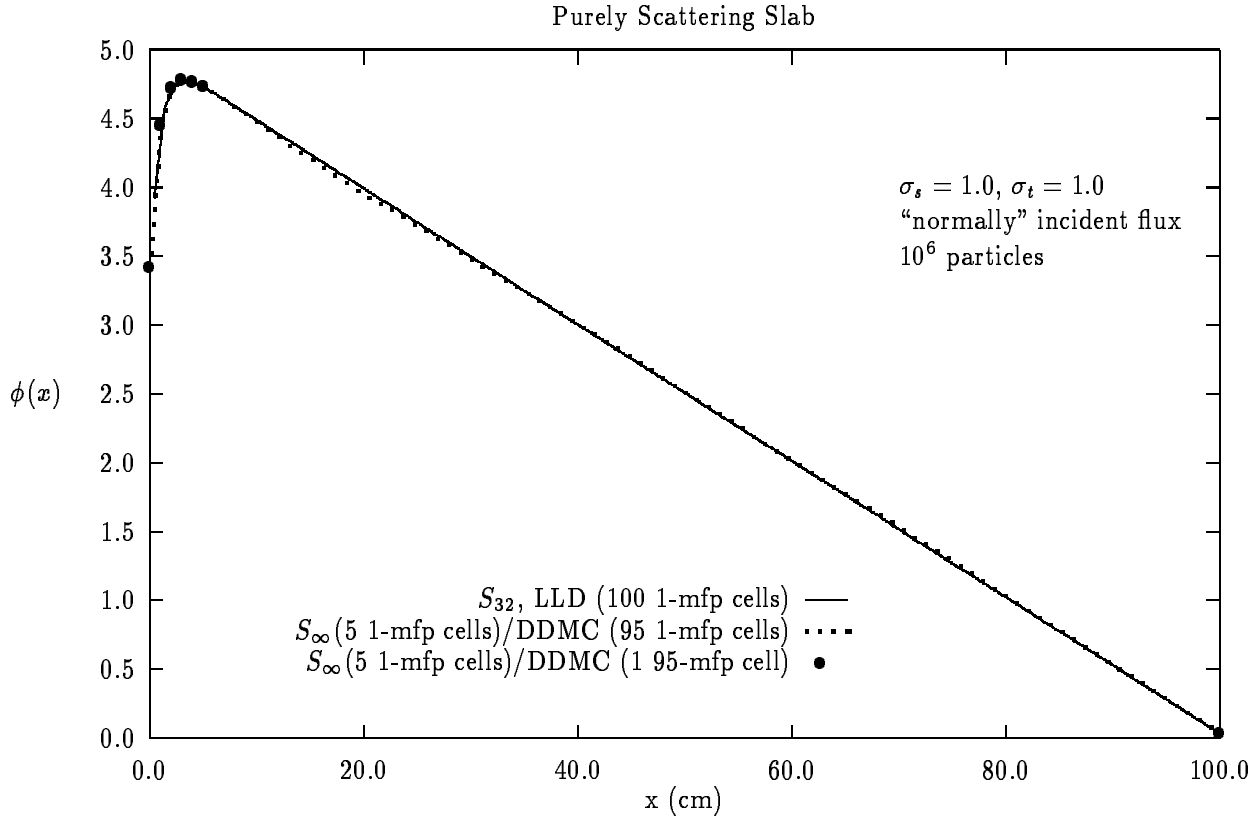

Figure 4: Multi-Hybrid (S_∞ and DDMC) results with different zoning of diffusion cells compared to S_∞ results.

and its discretization are described in Table 2. This problem tests a method's ability to model systems with large amounts of scattering. It also tests strong interface conditions where the scattering ratio is close to 1.0 (i.e., transport effects inside diffusive regions).

Table 2: Physical description of the McCoy and Larsen test problem.

	$0 < x < 12$cm	$12 < x < 15$cm	$15 < x < 21$cm	$21 < x < 30$cm
σ_t	3.33	3.33	1.33	3.33
σ_s	3.31002	3.31002	1.10523	3.31002
q^A	1.0	0.0	0.0	0.0
Δx	1.5	1.5	1.5	1.5

We take the S_{32}, LLD results as "truth." To those results we compare pure DDMC, pure S_∞, and Multi-Hybrid with S_∞ in the four cells between 10.5 and 16.5 cm and DDMC everywhere else. All results, except for the S_∞ results, are shown in Fig. 5. Except around 15.0 cm, the results agree fairly well.

For this problem, we incorporate the qualitative nature of the solution into the FOM by replacing the maximum statistical relative error, R_{max}, with the relative error with respect to the S_{32}, LLD scalar flux immediately to the right of 15.0 cm, a location with transport effects. We call this the FOM_{LLD} and tabulate it in Table 3. The Multi-Hybrid FOM_{LLD} is 2.7 times larger than the S_∞ FOM.

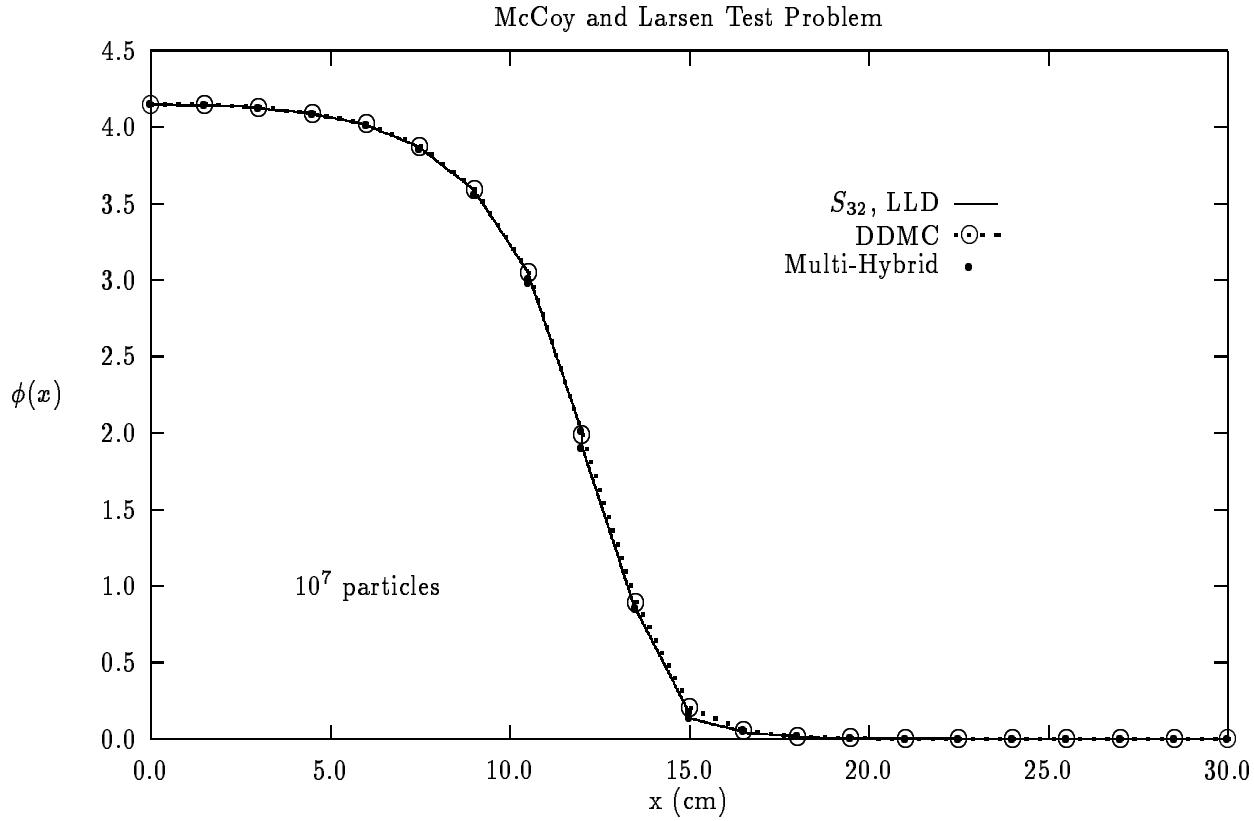

Figure 5: S_{32} LLD, DDMC, and Multi-Hybrid on the McCoy/Larsen Test Problem.

Table 3: Fluxes, times, and Figures of Merit for the McCoy/Larsen Test Problem.

Method	$\phi(15^+)$	t_{cpu} (s)	$\text{FOM}_{\text{LLD}}(15^+)$
S_{32}, LLD	0.13700		—
S_∞	0.13664 ± 0.00026	7095	20.4
DDMC	0.20068 ± 0.00026	813	0.0057
Multi-Hybrid	0.13745 ± 0.00035	1683	55.1

7 Conclusion

We have taken the principle behind the S_∞ method, replaced the transport with diffusion, and produced a Discrete Diffusion Monte Carlo (DDMC) hybrid method. This hybrid method gives results that agree well with deterministic, cell-centered diffusion results. With DDMC verified, we look ahead to using DDMC with residual methods in an attempt to achieve exponential convergence.

Since both the S_∞ and the DDMC methods are particle-based, we further combine them to obtain a Multi-Hybrid particle-based method. Any given cell may handle particles with either transport or diffusion, whichever is appropriate. We observed factors of 3 and 8 improvement in the Figures of Merit over pure S_∞.

Acknowledgments

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References

[Pomraning and Foglesong, 1979] G. C. Pomraning and G. M. Foglesong, Transport-Diffusion Interfaces in Radiative Transfer, Journal of Computational Physics, 32, pages 420-436 (1979).

[N'Kaoua, 1991] T. N'Kaoua, Solution of the Nonlinear Radiative Transfer Equations by a Fully Implicit Matrix Monte Carlo Method Coupled with the Rosseland Diffusion Equation Via Domain Decomposition, SIAM J. Sci. Stat. Comput., Vol 12, No. 3, pages 505-520 (1991).

[Fleck and Canfield, 1984] J. A. Fleck, Jr. and E. H. Canfield, A Random Walk Procedure for Improving the Computational Efficiency of the Implicit Monte Carlo Method for Nonlinear Radiation Transport", Journal of Computational Physics, 54, pages 508-523 (1984).

[Urbatsch, Morel, and Gulick, 1999] Todd J. Urbatsch, Jim E. Morel, and John C. Gulick, Monte Carlo Solution of a Semi-Discrete Transport Equation, Part I: Transport, these proceedings (1999).

[Halton, 1994] John H. Halton, Sequential Monte Carlo Techniques for the Solution of Linear Systems, Journal of Scientific Computing, Vol. 9, No. 2 (1994).

[Bell and Glasstone, 1985] George I. Bell and Samuel Glasstone, Nuclear Reactor Theory, Reprint by Robert E. Krieger Publishing Company, Malabar, Florida (1985).

[McCoy and Larsen, 1971] D. R. McCoy and E. W. Larsen, Unconditionally Stable Diffusion-Synthetic Acceleration Methods for the Slab Geometry Discrete Ordinates Equations. Part II: Numerical Results, Nuclear Science and Engineering, Vol. 82, pages 64-70 (1982).